

Numerical evaluation of the dipole-scattering model for the metal-insulator transition in gated high mobility Silicon inversion layers

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The dipole trap model is able to explain the main properties of the apparent metal-to-insulator transition in gated high mobility Si-inversion layers. Our numerical calculations are compared with previous analytical ones and the assumptions of the model are discussed carefully. In general we find a similar behavior but include further details in the calculation. The calculated strong density dependence of the resistivity is not yet in full agreement with the experiment.

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I. INTRODUCTION

Since its discovery in 1995¹, the metal-insulator transition in two dimensions (2D) was investigated carefully², as its finding is in apparent contradiction to the scaling theory of localization³. According to the latter, in the limit of zero temperature, a metallic state exists only in three dimensions, but in two dimensions disorder should always be strong enough in order to lead to an insulating state³. Nevertheless, high-mobility n-type silicon inversion layers showed for high electron densities a strong decrease of resistivity ρ towards temperatures below a few Kelvin, manifesting the metallic region, and a strong exponential increase of the ρ for low densities demonstrating the insulating regime. A very similar behavior was observed in many other semiconducting material systems at low temperatures.

After the unexpected finding, several models were suggested in order to explain the metallic behavior in 2D. The most important ones are i) temperature-dependent screening^{4,5,6}, ii) quantum corrections in the diffusive regime^{7,8,9}, iii) quantum corrections in the ballistic regime^{10,11}, and iv) scattering of electrons according to the dipole trap model¹². As there are argumentations for all that different models in the literature, we do not want to repeat them here in detail. A clear decision for one of the suggestions could not be drawn yet and further work on the models has to be carried out.

The dipole trap model was introduced by Altshuler and Maslov¹² (AM) especially for Si-MOS structures, as it is known that the misfit at the silicon/silicon-oxide interface produces charged defect states in the thermally grown oxide layer^{13,14,15}. AM could show that a hole trap level at energy E_t which is either filled or empty, depending on its position relative to the Fermi energy E_F , can lead to a critical behavior in electron scattering if E_t and E_F are degenerate.¹⁶ This dipole trap model can explain the main properties of the metal-insulator

transitions in gated Si-MOS structures¹².

In this work, we present numerical calculations of the temperature and density dependent resistivity due to electronic scattering in the dipole trap model. With these calculations we are able to check the analytical calculations with its approximations. Due to the numerical procedure, we can include further details and investigate their influence.

For the analytical calculations AM made a number of assumptions. These are: a1) the trap states possess a δ -like distribution in energy, a2) the spatial distribution in the oxide is homogeneous, a3) the occupied states behave neutral and cause no scattering of 2D electrons whereas the unoccupied states are positively charged and lead to scattering (hole trap), a4) a charged trap state is effectively screened by the 2D electrons so that the resulting electrostatic potential can be described by the trap charge and an apparent mirror charge with opposite sign on the other side of the interface, a5) the scattering efficiency of the 2D electrons is described by a dipole field of the trap charge and its mirror charge, a6) a parabolic saddle point approximation for the total potential of the trap states was used in order to perform analytical calculations, a7) the energy of the trap state E_{t0} is fixed relative to the quantization energy E_0 of the 2D ground state inside the inversion potential, and a8) the Fermi energy E_F in the 2D layer is either independent of or is the same as in the 3D substrate.

In contrast to AM, our calculations were performed numerically, so that several limitations of their calculations could be dropped. Our improvements concern i1) the detailed spacial dependence of the electrostatic potential is taken into account instead of the parabolic saddle point approximation, i2) the energy of the trap state E_{t0} is fixed relative to the conduction band edge E_{CB} . As a result of our calculations, we find a similar behavior of the calculated resistivity as AM and we calculate in addition the density dependence of the resistivity.

According to the restricted space in the original AM work, some of the used equations were not derived there. We will discuss these equations and considerations in detail in the main part. For better readability of our paper, some details were put into appendices. Please note that

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we will use SI units throughout this work.

II. MODEL CONSIDERATIONS AND NUMERICAL CALCULATIONS

The misfit at the Si/SiO₂ interface layer leads to different kinds of defects and trap states^{13,14,15,17}. In the considered AM model it is assumed that a relative large number of hole trap states exists. If such a trap state captures a hole, it is positively charged, otherwise it is neutral. In Fig. 1 the trap state is depicted schematically.

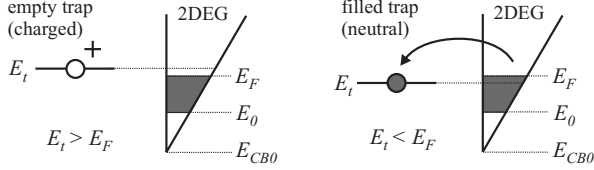


FIG. 1: Schematic representation of the trap state together with the 2D electron system (2DES). For $E_t > E_F$ the trap state is positively charged and scatters electrons in the 2D layer whereas for $E_t < E_F$ the trap is neutral, i.e. it is occupied with an electron and does not act as a scattering center. Note that the main recharging effect comes from the energetic position E_t of the trap state. It varies strongly with the applied gate voltage V_g , whereas the Fermi-energy E_F shows only small variations with changing electron density on the same scale.

As described in the introduction, it is further assumed that a1) all trap states exist at the same energy E_{t0} if no external field is applied and posses a2) a spatially homogeneous density distribution in the oxide layer. But a potential gradient due to an applied gate voltage V_g causes a linear increase of the trap energy position $E_t = E_{t0} + eV_g z/d$, where z is the distance from the Si/SiO₂ interface ($z < 0$) and d is the distance between gate electrode and that interface (i.e. the thickness of the oxide layer).

For the electrostatic potential inside the oxide layer, also the screening effects of the inversion layer have to be taken into account. For 2D electrons in a Si-(001) layer, the screening radius is equal to $a_B/4$. If the trap distance from the interface $|z|$ exceeds the screening radius, the in-plane components of the electrostatic field caused by the charged trap will effectively be screened. In that case, the electric field and the potential in the oxide can be described by the trap charge and an apparent mirror charge with opposite sign on the other side of the interface (assumption a4). The potential of the charged state caused by the image charge is $\Phi = e/(2 \cdot 4\pi\epsilon_0\epsilon_{ox}z)$ in SI units with $\epsilon_0 = 8.854 \times 10^{-12} \text{ Fm}^{-1}$ and $\epsilon_{ox} \approx 3.9$, the relative dielectric constant of the oxide. Thus the total energy of the charged trap state can be given as

$$E_t(z) = E_{t0} + eV_g \frac{z}{d} + \frac{e^2}{8\pi\epsilon_0\epsilon_{ox}z} \quad \text{for } z < 0. \quad (1)$$

The last term in Eq. 1 leads to a down bending of the energetic position towards the interface and causes a maximum in the total trap energy $E_t(z)$ as shown in Fig. 2.

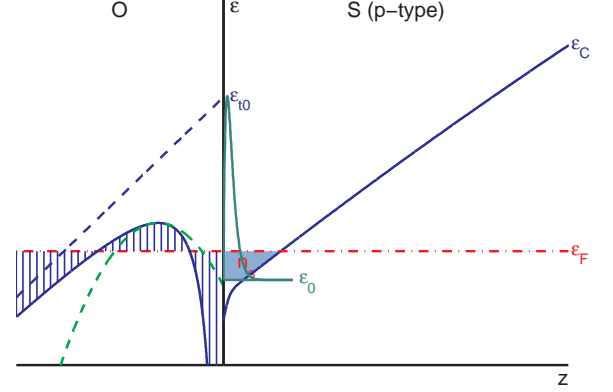


FIG. 2: Schematic representation of energies in the dipole trap model. The dashed blue line on the left represents the trap energy without, the full blue line with mirror charge potential. Note that the distance scale on the left and right hand side of the interface is chosen differently in order to increase visibility.

The trap charge together with its mirror charge form a dipole perpendicular to the interface plane. Thus, for distances larger than $2|z|$, the scattering potential experienced by the 2D electrons can be described by a dipole field which falls off with $1/r^3$ (assumption a5). This is in agreement with the long range field of a screened Coulomb potential in two dimensions and leads to a consistent description. AM have calculated the classical scattering cross section for momentum relaxation $\sigma_m(E, z)$ for such a dipole field for electrons with kinetic energy E as

$$\sigma_m(E, z) = 2.74(e^2 z^2 / 8\pi\epsilon_0\epsilon^* E)^{1/3} \quad (2)$$

with $\epsilon^* = (\epsilon_{ox} + \epsilon_{Si})/2 \approx 7.9$, the effective dielectric constant for the 2D electron system (2DES).

Whether a trap state is charged or not, depends on its energetical position relative to the Fermi energy E_F (assuming thermal equilibrium for the occupation). The occupation function corresponds to a modified Fermi-Dirac distribution, where the degeneracy of empty and filled states is taken into account. AM have assumed that the (positively) charged trap state can have either spin up or down and is thus doubly degenerate, while the neutral state has no degree of freedom and is not degenerate. From that the probability of a trap state to be charged follows as

$$p^+(z) = \frac{1}{1 + \frac{1}{2} \exp\left(\frac{E_F - E_t(z)}{kT}\right)} \quad (3)$$

with k the Boltzmann constant.

For the occupation of the trap states only the relative position of the trap energy $E_t(z)$ to the Fermi energy E_F is important. But the difference $E_F - E_t(z)$ can not be derived directly – it has to be calculated from the two individual energies which depend on different variables. According to Eq. 1, the z -dependence of the trap energy can be calculated, but one has to fix it's zero-position E_{t0} . AM have assumed (a7) a fixed energetical distance of the trap state relative to the quantization energy E_0 of the electronic ground state in the (nearly triangular) inversion potential. But E_0 depends on the strength and shape of the inversion potential and via electron-electron interaction on the 2D electron density n_s . Thus it seems not realistic that the energy of the trap state is fixed relative to E_0 , but rather that it is fixed relative to the energetic position of the conduction band edge E_{CB} (which is our improvement i2).

Equation 1 can be used as given, by noting that the energy is defined relative to the conduction band edge E_{CB} . On the other hand the ground state energy E_0 has to be calculated for the inversion potential, which itself depends on n_s and the depletion charge N^- and by including the electron-electron interaction¹⁴. As $E_F - E_0$ follows from the electron density n_s ¹⁸, together with E_0 one gets the position of E_F relative to the conduction band edge and the difference $E_F - E_t(z)$ can be used for $p^+(z)$ in Eq. 3.

In the Drude-Boltzmann approximation, the electrical resistivity ρ , equal to the inverse conductivity σ

$$\rho = \frac{1}{\sigma} = \frac{m^*}{ne^2} \frac{1}{\bar{\tau}} \quad (4)$$

follows by calculating the effective transport scattering time $\bar{\tau}$. The detailed calculation is performed in Appendix A.

As a result one gets that

$$\frac{1}{\bar{\tau}} = N_{\text{eff}}^+ v(\bar{E}) \sigma_m(\bar{E}, z_m), \quad (5)$$

can be expressed by the effective values N_{eff}^+ for the number of charged trap states per area, $v(\bar{E})$ the electron velocity, $\sigma_m(\bar{E}, z_m)$ the scattering cross section, and the average electron energy \bar{E} as given in Appendix A. These effective values depend on all the important variables of the systems, i.e. on T , V_g and so on. By inserting Eq. 5 into Eq. 4, one gets already the dependence of the resistivity ρ on the different parameters

$$\rho = \frac{m^*}{ne^2} N_{\text{eff}}^+ v(\bar{E}) \sigma_m(\bar{E}, z_m), \quad (6)$$

and we have verified equation Eq. 7 in Ref. 12.

From here our treatment of the subject is quite different from that of AM¹². They have evaluated Eq. 6 analytically whereas we perform the calculation of it numerically. But in order to be able to solve Eq. 6, AM have used a parabolic (saddle-point) approximation for the z -dependence of the trap energy (assumption a6).

The analytical expression of AM (Eq. 9) contains a temperature independent prefactor ρ_0 and a temperature dependent scaling function $R(V_g, T)$. For their case (A) of the temperature dependence of E_F , they get a critical behavior with $R(T)$ increasing for $V_g > V_g^c$ and decreasing for $V_g < V_g^c$ (see Fig. 1 in Ref. 12), similar to what is observed experimentally. For their case (B), $R(T)$ is always increasing with temperature and no critical behavior comes out.

In our numerical evaluation of Eq. A6, we use the exact dependence of $E_t(z)$ as given by Eq. 1 (our improvement i1). The numerical treatment prevents errors due to the parabolic approximation, but enables us also to include further details, which also cannot be solved analytically.

AM have calculated the temperature dependence of the resistivity in close vicinity of the critical density where the behavior changes from metallic to insulating behavior. We have calculated also the direct density dependence over a larger range for different temperatures. Fig. 3 shows how the effective number of charge trap states N_{eff}^+ depends on n_s .

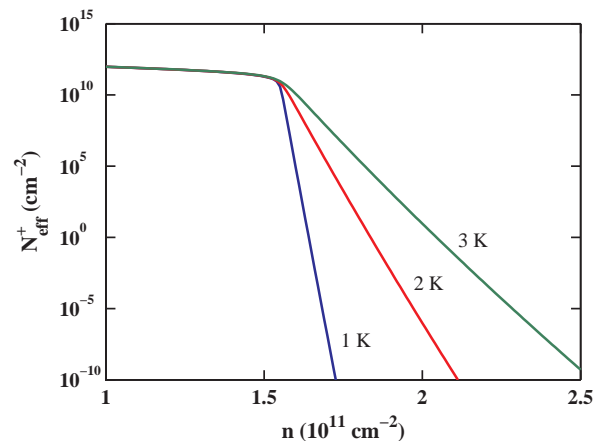


FIG. 3: Effective number of charged trap states per area N_{eff}^+ vs. electrons density (i.e. varying gate voltage) at temperatures of $T = 1, 3$, and 5 K.

As can be seen there is a very strong variation above $n_s \approx 1.5 \times 10^{11} \text{ cm}^{-2}$, where the maximum of the trap energy $E_t(z)$ is just degenerate with E_F . This strong variation comes from the fact that as soon as the maximum of $E_t(z)$ is below E_F only an exponentially small number of traps is still excited (i.e. charged) and the scattering efficiency decreases accordingly. As ρ is nearly proportional to N_{eff}^+ , such strong variations have not been observed experimentally. This discrepancy to the experiment can possibly be explained that in real 2D Si-MOS structures either the trap states do not have a δ -like distribution in energy or that in addition other scattering sources exist.

III. CONCLUSIONS

We have shown that the numerical calculations of the temperature dependent resistivity give similar results as the analytical methods by AM. The strong density dependence of N_{eff}^+ and thus of ρ which follows from the calculation is not in agreement with experimental findings. In order to possibly resolve this discrepancy further calculations should be performed within the dipole trap model. The numerical procedure allows incorporation of further effects and realistic assumption like energetical broadening of the trap level, special spatial distributions of the defects, and detailed screening dependence.

Acknowledgments

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APPENDIX A: TRANSPORT EQUATIONS

The effective transport scattering time $\bar{\tau}$ in the Drude-Boltzmann approximation follows from^{14,19}

$$\bar{\tau} = \frac{\int dE \tau(E) E \partial f / \partial E}{\int dE E \partial f / \partial E}, \quad (\text{A1})$$

with $\tau(E)$ being the energy dependent scattering time and $\partial f / \partial E$ the first derivative of the Fermi-Dirac distribution function f .

The transport scattering time $\tau(E)$ has to be calculated by integration over the individual scattering rates

$$1/\tau(E) = \int_0^d dz N_{t3}^+(z) v(E) \sigma_m(E, z) \quad (\text{A2})$$

with the density of charged traps $N_{t3}^+(z) = N_{t3} P_+(z)$, N_{t3} the spatially constant density of existing trap states

(both being three dimensional volume densities) and $v(E)$ the electron velocity.

By inserting the all expressions into Eq. A2 one gets

$$1/\tau(E) = c' N_{\text{eff}}^+ z_m^{2/3} E^{1/6} \quad (\text{A3})$$

with the prefactor $c' = 2.74(e^2/8\pi\epsilon_0\epsilon^*)^{1/3}\sqrt{2/m^*}$, an effective number of positive trap states per area $N_{\text{eff}}^+ = N_{t3} \langle \Delta z \rangle_{\text{eff}}$, the effective width of positive charge layer $\langle \Delta z \rangle_{\text{eff}} = \int dz p_+(z)(z/z_m)^{2/3}$ and the position $z_m = \sqrt{ed/8\pi\epsilon_0\epsilon_{ox}V_g}$ of the energetical maximum of the trap energy.

By inserting Eq. A3 into Eq. A1, one gets

$$\bar{\tau} \propto 1/E_F \int_0^\infty dE E^{5/6} \partial f / \partial E. \quad (\text{A4})$$

Further an effective energy \bar{E} can be defined so that formally Eq. A3 can be preserved for the effective $\bar{\tau}$, i.e. $1/\bar{\tau} = c' N_{\text{eff}}^+ z_m^{2/3} \bar{E}^{1/6}$. A simple calculation gives

$$\bar{E} = E_F \left[\int_0^\infty dE \left(\frac{E}{E_F} \right)^{5/6} \partial f / \partial E \right]^{-6}. \quad (\text{A5})$$

By further replacing the first derivative of the Fermi-Dirac function by the identity $\partial f / \partial E = -f(1-f) = -(4kT \cosh^2((E-E_F)/2kT))^{-1}$ one obtains the same expression as Eq. 8 in Ref. 12.

With these relations, the resistivity can exactly be written in terms of the effective energy \bar{E} as

$$\rho = \frac{m^*}{ne^2} N_{\text{eff}}^+ v(\bar{E}) \sigma_m(\bar{E}, z_m), \quad (\text{A6})$$

which corresponds to Eq. 7 in Ref. 12, but the individual terms are rewritten according to our definitions above. A comparison with Eq. 4 gives exactly

$$\frac{1}{\bar{\tau}} = N_{\text{eff}}^+ v(\bar{E}) \sigma_m(\bar{E}, z_m), \quad (\text{A7})$$

and shows that Eq. A2 can also be rewritten for effective values.

¹ S.V. Kravchenko, et al. Phys. Rev. B **50**, 8039 (1994); Phys. Rev. B **51**, 7038 (1995).

² for a review see e.g. S.V. Kravchenko and M.P. Sarachik, Rep. Prog. Phys. **67**, 1 (2004).

³ E. Abrahams, P. W. Anderson, D. C. Licciardello, and T. V. Ramakrishnan, Phys. Rev. Lett. **42**, 673 (1979).

⁴ F. Stern, Phys. Rev. Lett. **44**, 1469 (1980).

⁵ A. Gold and V.T. Dolgoplov, Phys. Rev. B **33**, 1076 (1986).

⁶ S. Das Sarma, Phys. Rev. B **33**, 5401 (1986).

⁷ A.M. Finkelstein, Z. Phys. B: Condens. Matter **56**, 189 (1984).

⁸ C. Castellani, C. Di Castro, P. A. Lee, and M. Ma, Phys. Rev. B **30**, 527 (1984).

⁹ A. Punnoose and A.M. Finkelstein, Phys. Rev. Lett. **88**, 016802 (2002).

¹⁰ G. Zala, B.N. Narozhny, and I.L. Aleiner, Phys. Rev. B **64**, 214204 (2001).

¹¹ I.V. Gornyi and A.D. Mirlin, Phys. Rev. B **69**, 045313 (2004).

- ¹² B. L. Altshuler and D. L. Maslov, Phys. Rev. Lett. **82**, 145 (1999).
- ¹³ “*Physics of Semiconductor Devices*”, S. M. Sze, John Wiley & Sons, New York 1981, p. 379.
- ¹⁴ T. Ando, A. B. Fowler, and F. Stern, Rev. Mod. Phys. **54**, 437 (1982).
- ¹⁵ “*Gate Dielectrics and MOS ULSIs*”, T. Hori, Springer Verlag, Berlin, 1997.
- ¹⁶ Note: In this work we use a temperature dependent Fermie energy $E_F(T)$ instead of the chemical potential $\mu(T)$ in contrast to AM, who used the nomenclature of E_F beeing identical to the chemical potential μ at $T = 0$ and using the chemical potential $\mu(T)$ for any higher temperature.
- ¹⁷ Note: The type of trap states considered by AM might correspond to Si–Si weak bonds, which act like donors, i.e. being either neutral or positively charged. If the energetic position is deep inside the energy gap, it can also be seen as a hole trap state.
- ¹⁸ Note: In this work we calculate the Ferme energy inside

the 2D layer according to the electron density n_s . AM have considered two different cases in their work, the one discussed before is their case (B), whereas their case (A) assumes that the Fermi energy (chemical potential) of the 2DES and the Si substrate coincide and show the same temperature dependence. We do not consider case (A) in detail, as we think that case (B) is more realistic.

- ¹⁹ Note: The weighting of $\tau(E)$ with the kinetic electron energy E in Eq. A1 fundamentally follows from the Drude-Boltzmann approximation²⁰ as the Fermi velocity v_F and the shift of the Fermi surface in k-space are both proportional to \sqrt{E} , which enter into the expression for the current $j_x = -e \int d\vec{k} n(\vec{k}) f(E) v_x$. The integral in the denominator of Eq. A1 in 2D is just equal to the Fermi energy E_F — also for elevated temperatures.

- ²⁰ “*Semiconductors*”, R. A. Smith, Cambridge University Press, Cambridge 1964.